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From atomistic interfaces to dendritic patterns

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Transport processes around phase interfaces, together with thermodynamic properties and kinetic phenomena, control the formation of dendritic patterns. Using the thermodynamic and kinetic data of phase interfaces obtained on the atomic scale, one can analyse the formation of a single dendrite and the growth of a dendritic ensemble. This is the result of recent progress in theoretical methods and computational algorithms calculated using powerful computer clusters. Great benefits can be attained from the development of micro-, meso- and macro-levels of analysis when investigating the dynamics of interfaces, interpreting experimental data and designing the macrostructure of samples. The review and research articles in this theme issue cover the spectrum of scales (from nano- to macro-length scales) in order to exhibit recently developing trends in the theoretical analysis and computational modelling of dendrite pattern formation. Atomistic modelling, the flow effect on interface dynamics, the transition from diffusion-limited to thermally controlled growth existing at a considerable driving force, two-phase (mushy) layer formation, the growth of eutectic dendrites, the formation of a secondary dendritic network due to coalescence, computational methods, including boundary integral and phase-field methods, and experimental tests for theoretical models—all these themes are highlighted in the present issue.

This article is part of the theme issue 'From atomistic interfaces to dendritic patterns'.

Introduction

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1. Introduction

A complex tree-like structure containing the main stem and lateral branches is called a dendrite (from the Greek word δένδρον, dendron, 'tree'; figure 1) [2,3]. Dendritic structures control the properties of a broad range of advanced materials and arise during the different phase and structural transformation processes (ranging from materials physics to life sciences) and in many natural phenomena. For instance, crystal growth in liquids, domain evolution in ferroelectrics, lava crystallization on the outer surface and at the boundary of the Earth's inner core, freezing of sea ice in polar regions, solidification of superalloys and two-dimensional materials, crystallization of silica micelle structures and biological proteins, and the production of food, pharmaceuticals and speciality chemicals—all these processes and phenomena evolve with dendrite pattern formation [4–15].

Besides the first analytical models that described the shape of needle-like crystals [16–19] and that enabled the velocity of the dendrite and its tip radius to be obtained [3,20], the numerical study of dendrites began with cellular automata models [21,22], phase-field models [23] and the boundary integral method [24]. Owing to good knowledge of interfacial anisotropy, well-developed algorithms and powerful computers, it will soon be possible to model the fine patterns in snowflakes, hollow prisms, plates, columns and needles [25].

As confirmed by experiments and modelling results [26], dendrite formation is controlled by both mesoscale diffusive–convective heat-mass transport and capillary forces, which act at the atomic scale (comparable to a nanometre-wide solid–liquid interface). This is why the evolution of mesoscopic and macroscopic dendritic patterns must be studied with atomistic modelling. At the atomic level, both molecular dynamics and Monte Carlo simulations play important roles in determining the necessary interfacial parameters and their associated anisotropies. In parallel with these atomistic simulations, the phase-field approach has been detailed as the most thermodynamically consistent method for modelling dendritic growth and the evolution of other possible microstructures [27,28]. Linking atomistic and mesoscopic phase-field modelling quantitatively improves the interpretation of experimental results [29,30].

In this theme issue, a whole spectrum of dendritic pattern evolution, ranging from the atomic level of newly born crystals to their growth at the mesoscopic level, and finally to macroscopic pattern formation, is demonstrated. Authors in this issue have contributed to the studies of different scales of pattern evolution. The phase-field crystal (PFC) method is used at the atomic level, the solvability theory and traditional phase-field approach are presented at the mesoscopic scale, and, finally, the mushy layer theory, boundary integral method and stability theory allow us to analyse dendritic ensembles at the macroscopic level.

2. Fields and methods

To give a picture of micro-, meso- and macro-lengths in interface dynamics, various models and advanced methods are included in this theme issue. At the microscale, continuous atomistic models, such as the PFC model, which pertains to a continual atomic description at the level of atomic density distribution, are presented. At the mesoscale, advanced phase-field methods (based on the Landau theory of phase transitions) and morphological stability analysis are used. At the macroscale, theoretical and computational methods, developed using boundary integral methods and the theory of the two-phase (mushy) layer, are presented to describe the behaviour of dendrites and dendritic ensembles.

(a) Microscopic description and analysis of interfacial patterns

A microscale level of description is directly connected to the atomistic model that is based on the continuous PFC method. In relation to this topic, Provatas and co-workers [31] analyse the process of gas porous formation in the liquid–solid environment of inter-dendritic space during the last stages of solidification. Although such a process is well known from earlier experiments and has

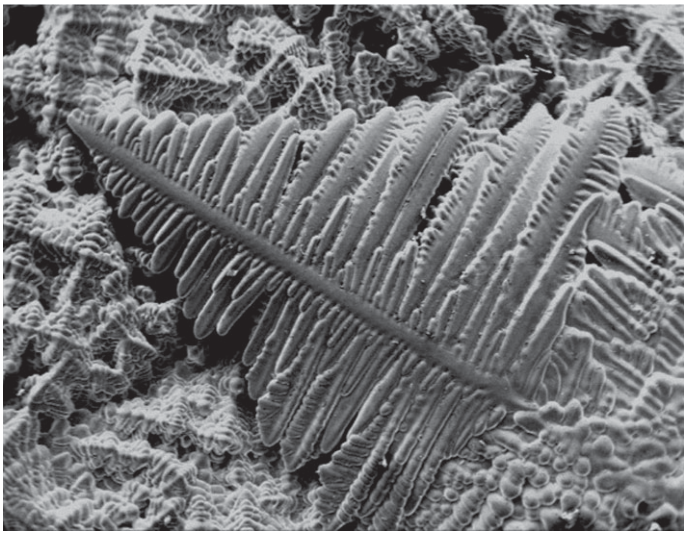

Figure 1. Electron micrograph of a dendritic crystal in a solidified metallic sample processed by an electromagnetic levitator [1]. The dendrite central trunk is 100 μm long.

been studied within continuous-based models, the motivation for this work was to provide an analysis at the atomistic level (figure 2). With this aim, the authors used the multi-PFC model, which describes the considered three-phase mixture at the level of atomic density. The model is able to describe a liquid pressure drop and the cavity pressure due to solidification shrinkage that also captures the Scheil–Gulliver-type segregation behaviour. As a result, the authors show that one can predict defects at the atomic level—a task that has direct practical importance and that is an undoubted merit of this work.

Smoothing over the periodic atomistic profile one can transfer to the envelope of maxima of atomic density. Such a multi-scale procedure [33] leads to the amplitude equations that describe the mesoscopic phase-field dynamics. Nizovtseva & Galenko [34] describe the amplitude dynamics via travelling waves. Using the analytical tanh method, the obtained set of travelling wave solutions describes the profiles, self-consistent velocity and correlation length of amplitudes. These solutions can also be used for estimations of the interface dynamics of dendritic patterns.

Using the non-Markovian master equation and memory functions, Jou & Galenko [35] offer a special method based on averaging microscopic (atomistic) ensembles. Their work is devoted to the slow and rapid transitions between metastable and (meta)stable states, which are described using the generalized hydrodynamics and thermodynamics of irreversible processes [36]. As is shown, the use of exponential memory leads to the hyperbolic phase-field model of the C-class, which is suitable for rapid solidification [37]. While complementary to some other approaches (e.g. volume averaging or multi-scale analysis applied to the classical density functional theory type-theories), the present coarse-graining approach for deriving phase-field models, however, offers a novel insight into the stochastic processes occurring at the atomic scale, through the transition probabilities of microscopic states. This is especially valuable when considering the separation of noise from the free energy, as in [38].

Two principally new and unusual tasks finalize this topical section. These are directly attributed to pattern formation of graphene islands in two-dimensional films by Elder *et al.* [39] and exotic dendrites in ferroelectrics by Shur & Akhmatkhanov [40]. Using the two-dimensional PFC model, Elder *et al.* reproduce the phenomenon of disappearance of graphene flakes due to hydrogen gas pressure. The results of the experimental study on domain shape instabilities and self-similar domain structures in several uniaxial ferroelectrics are summarized by Shur and Akhmatkhanov. It is very remarkable that both of these nano-scaled studies exhibit sixfold

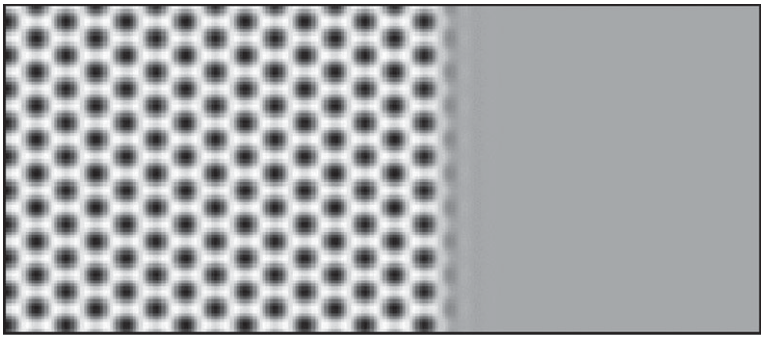

Figure 2. The phase interface at the scale of the atomic density distribution. Here, the two-dimensional sample front between the crystalline periodic triangular pattern (left) and the homogeneous liquid (right) are shown as the result of PFC modelling [32].

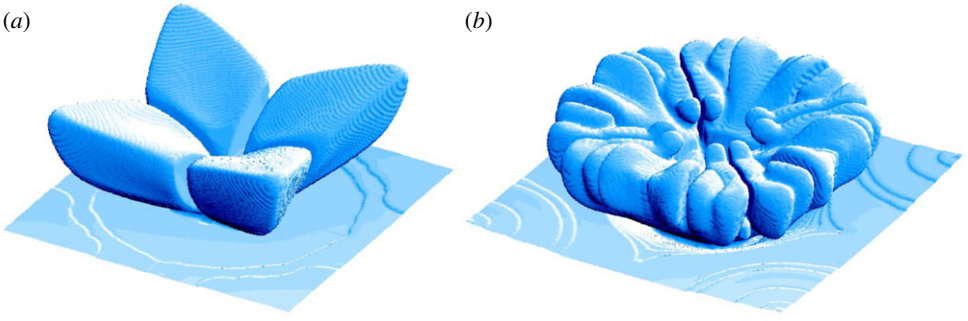

Figure 3. Crystal 'flowers on the lawn' obtained by phase-field modelling (PK Galenko 2004, unpublished results). (*a*) The crystal as a dendritic flower has grown due to large interface anisotropy. (*b*) The crystal as a fractal flower has grown due to zero interface anisotropy. (Online version in colour.)

symmetrical dendrites in two-dimensional samples. A stable growth mode in the selection of graphene and ferroelectric (niobate(tantalite)-lithium) dendrites might be further analysed for comparison of their formation with the already known regimes of dendrites growing from vapour or liquids.

(b) Experimental study and mesoscopic modelling of dendrites

The growth of dendrites is controlled by heat and mass transport in volumes of samples and the anisotropic properties of the phase interface (figure 3). An analysis of dendritic patterns developing at the meso-scale is offered by both the theoretical and experimental works.

The growth of semiconductor dendrites is analysed by Herlach *et al.* [41] through the measurement of crystal growth dynamics in the Ge, Si and $Ge_{100-x}Si_x$ ($x = 25$, 50, 75) melts as a function of undercooling. The authors offer a short but comprehensive overview on the kinetic mechanisms of growing crystals. The measured growth velocity and obtained microstructure of the solidified samples allow the sharp interface model predictions to be verified and provide tests of the current theory of dendritic growth at the mesoscopic length scale.

The effect of convective flow on dendrite formation is examined by Pericleous and co-workers [42] through the analysis of the thermoelectric magnetohydrodynamic (TEMHD) effect, which demonstrates that the dendrite tip velocity during growth from an undercooled melt is functionally dependent on the magnetic field. Indeed, the dendrite velocity has a retrograde behaviour as the magnetic field intensity increases from 0 to 6 T. Numerical simulations indicate that the overall microstructure is also significantly modified due to the TEMHD effect. The

magnetic field damps convection in the bulk liquid away from the solidification front, but, in contrast, it drives the flow through the inter-dendritic space. Such microstructure evolution in a solidifying undercooled droplet is investigated for a range of magnetic field strengths.

The growth of eutectic structures is analysed by Gao [43] within the concept of eutectic dendrites, which are characterized by a nearly flat solid–liquid interface but with a dendritic contour related to a negative thermal gradient ahead of the solidification front. With this idea, a free eutectic growth model is proposed in which the stability criterion established for the three-dimensional dendritic growth of a single phase at arbitrary Péclet numbers is applied to the tip stability of the dendritic contour. The model is tested using the recently measured growth velocities of eutectic dendrites in undercooled Ni–Sn eutectic alloys.

Using the phase-field method, Cool & Voorhees [44] investigate the coarsening of dendrites in a Pb–Sn alloy upon primary solidification. The authors present the modelling results and give an analysis of dendrite arm coalescence, fission events and dendrite fragmentation with the formation of the secondary structure. As a whole, this work presents a successful attempt to demonstrate that the phase-field simulation captures the proper coarsening kinetics which is observed experimentally in samples processed on board the International Space Station.

In the review article written by the editors of this theme issue [45], the kinetics of thermo-solutal dendrites via theoretical modelling is analysed. An inclusion of the flow and physically relevant n-fold symmetry of the surface energy makes their analysis flexible enough to estimate the experimental data for various crystal growth conditions and different chemical compositions of solidified samples. In particular, the authors show the applicability of their solvability theory to the prediction of dendrite growth velocity during solidification of D_2O-water, succinonitrile under terrestrial and microgravity conditions, congruently melting alloy, undercooled nickel and titan–aluminium melts.

Rapid dendritic growth is a phenomenon in which the non-equilibrium effects play a special role in the formation of primary and secondary structures. Solute trapping and the disappearance of solute drag with the increase in crystal growth velocity lead to the formation of metastable structures in various solutions, organic mixtures, semiconductors, metallic and metal–metalloidal alloys. One of the non-equilibrium effects in a form of disorder trapping is analysed by Rettenmayr *et al.* [46] within the context of rapid dendritic crystallization. The developed phase-field model predicts the transition from ordered to disordered crystals as the solid–liquid interface velocity increases. In the example of a congruently melting alloy, these authors numerically show that the velocity may sharply change at some critical undercooling in qualitative consistency with the theory of kinetic phase transitions and experiments on dendrites rapidly growing from the undercooled intermetallic melts.

(c) The macroscopic modelling of dendrites and grains

The macro-level of dendrite formation is characterized by the origination of a two-phase (mushy) layer (figure 4). The mushy layer represents the heterogeneous region between a macroscopically homogeneous mother phase (usually liquid) and a homogeneous solid phase (usually an amorphous or crystalline phase). The formation of this region provides the quickest relaxation to equilibrium during the phase and/or structural transformation.

In the paper written by Makoveeva & Alexandrov [47], the structure and typical regions appearing in the mushy layer are discussed in detail. Furthermore, the authors analyse the process of nucleation and growth of newly born crystals in the most undercooled part of a mushy layer. Taking into account the presence of fluctuations in the growth rates of crystals, i.e. the so-called 'diffusion' term in the Fokker–Planck equation for the distribution function, as well as the mass sources (heat sinks) in the balance equation for system supersaturation (supercooling), they have obtained a complete analytical solution of the integro-differential model by means of the saddle-point technique for the Laplace-type integral.

The theory of a two-phase mushy layer is developed in the next paper [48], which is devoted to the evolutionary behaviour of directional solidification with nucleating crystals. In this

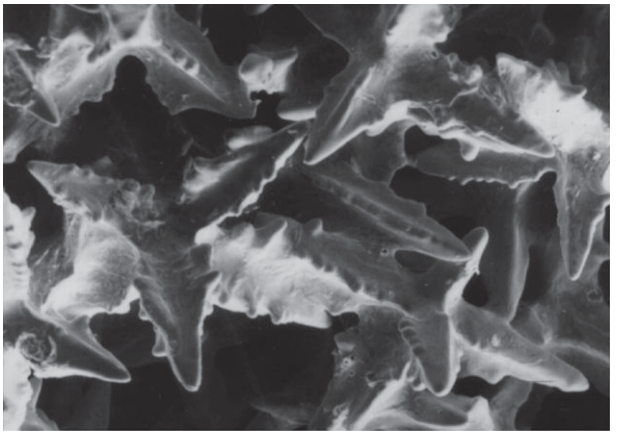

Figure 4. Dendritic ensemble within a two-phase mushy layer which represents the heterogeneous zone between a metastable liquid and a (meta)stable crystalline solid [22].

paper, a nonlinear system of governing equations representing the moving-boundary problem is formulated and solved analytically. The transient behaviour of the crystal size distribution function, temperature and concentration fields is analysed. The dynamical laws of motion of the nucleation front are found for kinetic and diffusionally controlled crystallization scenarios. The last two papers describe the evolutionary behaviour of the most undercooled part of a mushy layer, where nucleation and growth of crystals occur. The dynamical behaviour of the adjacent part of this layer, which is filled with dendrite-like structures, is analysed in the next paper [49].

Let us especially note that a number of crystallization processes occurring in nature and industry essentially depend on the stochastic fluctuations induced by different physical parameters (so, for instance, the atmospheric temperature fluctuations on the ice surface or the fluid velocity oscillations in the under ice oceanic boundary layer may be mentioned as such examples). The nonlinear dynamics of crystallization with a mushy layer under the influence of stochastic parameters is investigated in the paper presented by Ryashko and co-workers [49]. Here a pronounced effect of stochastic fluctuations (caused by the atmospheric temperature and fluid friction velocity) on the crystallization dynamics is studied. The rapid unpredictable stochastic changes in different system parameters lead to the unusual noise-induced solidification scenarios in the mushy layer as well as at its boundaries, 'solid phase–mushy layer' and 'mushy layer–liquid phase'. One of the main conclusions following from this research article consists in the fact that the presence of noise drastically changes the mushy layer dynamics compared with the classical deterministic scenario [50,51]. This paper presents an area of research in the nonlinear dynamics of crystallization processes—a phenomenon of stochastically induced shifts of different dynamical dependencies in a mushy layer.

The evolutionary theory of the curved solid–liquid interface, which, in many cases, precedes the mushy layer appearance, is analysed in the concluding overview [52]. In this paper, the boundary integral theory describing the propagation of arbitrarily curved phase interfaces is developed. Intrinsically, this theory gives the solution to the Stefan thermodiffusion problem with a curved solid–liquid interface in the form of a single integro-differential equation. The theory generalizes the evolutionary behaviour of slow (parabolic heat and mass transfer) and rapid (hyperbolic mass transfer) curvilinear fronts. The integro-differential equation for the interface function for solidifying binary non-isothermal mixtures is analysed. Analytically, a thermo-solutal selection criterion of the stable steady-state growth of dendrites is deduced. The computational modelling carried out on the basis of the boundary integral theory shows the selection of structures in the form of dendritic, fractal or planar crystals, which appear at different values of the undercooling.

3. Conclusion

In this theme issue, the multi-scale problems of moving interfaces with dendritic formations are considered, studied and discussed. New trends for creating efficient theoretical and computational models are shown. These models represent a step forward in terms of developing the efficient applicability of atomic and mesoscopic models for a broad range of materials, including semiconductors, metals, alloys, graphene, intermetallic, metalloid and ferroelectric compounds.

While new data on the multi-scale dendritic problem have been reported, including micro- and meso-lengths for defining the formation of dendritic patterns [53–56], the present theme issue presents a description of the two-dimensional dendrites forming in films of graphene and ferroelectrics, the latest stages of solidification with porous origination, dendritic coalescence near the equilibrium, morphological transitions at high growth rates, the influence of stochasticity on the formation of the two-phase mushy layer and the effect of convective flow on growth kinetics under microgravity and terrestrial conditions. The last is one of the fundamental problems of pattern formation on Earth and in space with application to novel materials development [26,57].

Finally, a general framework for truly satisfying scale-bridging theoretical models and experimental methods is still an open matter [58–60]. This theme issue attempts to bridge concepts and methods at different temporal scales and spatial lengths all together in order to achieve a meaningful potential in the aforementioned fields of materials science.

Data accessibility. This article has no additional data.

Competing interests. We declare we have no competing interests.

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